SACADA Database Code: 187

Topology: csp

# of independent nodes (IN): 3
Transitivity: [3774]
Space Group: Pm-3n
Pearson: cP120
Coordination Number (CN): 4

Year: 1991

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
csp (SACADA #187)		2.657		1.235	294.5	273.5	46.6	SACADA[1]
csp								doi: 10.1038/352674a0

Elasticity tensor (kBar)[1]

6888.9667	972.5160	972.5160	-0.0000	0.0000	0.0000
972.5160	6888.9667	972.5160	-0.0000	-0.0000	-0.0000
972.5160	972.5160	6888.9667	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	2597.2592	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	2597.2592	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	2597.2592

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].